Entropy-driven phase transitions in multitype lattice gas models

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February 23, 2000

In multitype lattice gas models with hard-core interaction of Widom–Rowlinson type, there is a competition between the entropy due to the large number of types, and the positional energy and geometry resulting from the exclusion rule and the activity of particles. We investigate this phenomenon in four different models on the square lattice: the multitype Widom–Rowlinson model with diamond-shaped resp. square-shaped exclusion between unlike particles, a Widom–Rowlinson model with additional molecular exclusion, and a continuous-spin Widom–Rowlinson model. In each case we show that this competition leads to a first-order phase transition at some critical value of the activity, but the number and character of phases depend on the geometry of the model. Our technique is based on reflection positivity and the chessboard estimate.

KEY WORDS: first-order phase transition, entropy-energy conflict, staggered phase, Widom–Rowlinson lattice gas, plane-rotor model, ferrofluid, percolation, chessboard estimate, reflection positivity.

1 Introduction

Although the most familiar examples of phase transitions in lattice models originate from a degeneracy of ground states and therefore occur at low temperatures, this is not the only situation in which phase transitions can occur. Another possible source of criticality is a conflict of energy and entropy. This was noticed first by Dobrushin and Shlosman [5] in the case of an asymmetric double-well potential with two (sharp resp. mild) local minima separated by a barrier. They found that for some specific temperature energy and entropy attain a balance leading to the coexistence of high- and low-temperature phases corresponding to the two wells; cf. also Section 19.3.1 of [8]. Later on, Kotecký and Shlosman [10] observed that such a first-order phase transition can occur even in the absence of an energy barrier, provided there is an "explosion" of entropy. They demonstrated this in particular on the prototypical case of the q-state Potts model on $\mathbf{Z}^d$ for large q, showing that for a critical temperature there exist

q distinct ordered low-temperature phases as well as one disordered high-temperature phase; see also Section 19.3.2 of [8].

This paper has the objective of studying entropy-driven first-order phase transitions of similar kind in multitype lattice gas models with type-dependent hard core interaction. In such models the crucial parameter is the activity instead of temperature, and the entropy-energy conflict turns into a competition between the entropy of particle types and the positional energy and geometry resulting from the exclusion rule and the activity of particles. One is asking for a critical activity with coexistence of low-density and high-density phases.

The basic example of this kind is the multicomponent Widom–Rowlinson lattice gas model investigated first by Runnels and Lebowitz [15] in 1974 and studied later (theoretically and numerically) by Lebowitz et al. [12], cf. also [13]. If the number q of types is large enough (the numerical estimates give $q \geq 7$), there exist three different regimes: besides the low-density uniqueness regime and a high-density regime with q "demixed" phases for $z > z_c(q)$, there exists an intermediate domain of activities $z_0(q) < z < z_c(q)$ with two "crystal" (or "staggered") phases with an occupation pattern of chessboard type, and the phase transition at $z_c(q)$ is of first order. The transition between staggered and demixed phases at $z_c(q)$ is again entropy-driven: in the staggered phases the type entropy wins, with the effect of an entropic repulsion of positions forcing the particles onto a sublattice, whereas in the demixed phases the particles gain energy and positional freedom but loose their type entropy. The same kind of phenomenon has also been discovered for a class of spin systems with annealed dilution (including diluted Potts and plane rotor models) [3, 4].

The aim of the present paper is to analyze the interplay of type entropy and the geometry induced by the lattice and the exclusion rule. While we stick to the integer lattice $\mathbf{Z}^d$ (and for simplicity in fact to the case $d = 2$), we vary the exclusion rule in order to gain some insight into the geometric effects involved. We investigate and compare four different models:

1. the standard multitype Widom–Rowlinson model;
2. a multitype Widom–Rowlinson model with nearest-neighbor and next-nearest neighbor exclusion between particles of different type;
3. a multitype Widom–Rowlinson model with additional type-independent hard-core interaction between next-nearest particles;
4. a ferrofluid model of oriented particles with exclusion between neighboring but not sufficiently aligned particles. (Similar continuous-spin counterparts of models 2 and 3 will also be considered.)

We show that in each of these examples an entropy-driven first-order phase transition occurs, but the number and specific characteristics of coexisting phases are different in all cases. Our technique is similar to that used in [3, 4, 5, 10] and Chapters 18/19 of [8], and is based on the (trivial) reflection positivity in lines through lattice sites and the resulting chessboard estimate [8]. While in model 1 this is only an alternative

(and perhaps more elementary) approach to the results obtained in [12] by means of Pirogov-Sinai theory, the very same argument works also in the other models with only slight modifications.

This paper is organized as follows. In Section 2 we introduce the four models and present our results. The proofs follow in Sections 3 to 6. The general scheme is explained in detail for model 1, the standard Widom–Rowlinson lattice model. In the other cases we only indicate the necessary changes.

Acknowledgement. H.O.G. gratefully acknowledges warm hospitality of the Centre de Physique Théorique in Marseille-Luminy, and V.Z. of the Mathematical Institute of the University of Munich. This work was supported by the Deutsche Forschungsgemeinschaft, SPP 1033.

2 Models and results

2.1 The multitype Widom–Rowlinson lattice gas

This model describes a system of particles of q different types ('colors') which are allowed to sit on the sites of the square lattice $\mathbf{Z}^2$. (For simplicity we stick to the two-dimensional case; an extension to higher dimensions is straightforward, cf. Chapter 18 of [8] or [7].) At each lattice site we have a random variable σ_i taking values in the set $E = \{0, 1, \ldots, q\}$. The equality $\sigma_i = 0$ means that site i is empty, and $\sigma_i = a \in \{1, \ldots, q\}$ says that i is occupied by a particle of color a. Particles of different color interact by a hard-core repulsion: they are not allowed to sit next to each other. There is no interaction between particles of the same color. This means that the formal Hamiltonian has the form

$$H(\sigma) = \sum_{\langle ij\rangle} U(\sigma_i, \sigma_j) \;, \tag{1}$$

where the sum extends over all nearest-neighbor pairs $\langle ij\rangle \subset \mathbf{Z}^2$ of lattice sites (i.e., $|i-j| = 1$), and the potential U is given by

$$U(\sigma_i, \sigma_j) = \begin{cases} \infty & \text{if } 0 \neq \sigma_i \neq \sigma_j \neq 0 \;, \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

This model is a lattice analog of the continuum two-species model of Widom and Rowlinson [16], and was first introduced by Lebowitz and Gallavotti [11] (for $q = 2$) and Runnels and Lebowitz [15] (for general q).

Since U is either 0 or ∞, the temperature does not play any role, and the only energetic parameter is the activity $z > 0$ which governs the overall particle density; we assume that the activity does *not* depend on the particle color. Accordingly, the Gibbs distribution in a finite region $\Lambda \subset \mathbf{Z}^2$ with boundary condition η in $\Lambda^c = \mathbf{Z}^2 \setminus \Lambda$ is given by

$$\mu^{z,q}_{\Lambda,\eta}(\sigma) = 1_{\{\sigma\equiv\eta \text{ off } \Lambda\}}\, (Z^{z,q}_{\Lambda,\eta})^{-1}\, z^{N_\Lambda(\sigma)} \exp\Big[-\sum_{\langle ij\rangle\cap\Lambda\neq\emptyset} U(\sigma_i, \sigma_j)\Big] \;, \tag{3}$$

where $N_\Lambda(\sigma) = |\{i \in \Lambda : \sigma_i \neq 0\}|$ is the number of particles in Λ, and $Z^{z,q}_{\Lambda,\eta}$ is a normalizing constant.

Alternatively, we may think of $\mu^{z,q}_{\Lambda,\eta}$ as obtained by conditioning a Bernoulli measure on the set of admissible configurations. Let

$$\Omega = \{\sigma \in E^{\mathbf{Z}^2} : \forall \langle ij \rangle \ \sigma_i \sigma_j = 0 \text{ or } \sigma_i = \sigma_j\}$$

be the set of all admissible configurations on $\mathbf{Z}^2$. Given any such configuration $\sigma \in \Omega$ and any subset Λ of $\mathbf{Z}^2$, we write σ_Λ for the restriction of σ to Λ. We also write $\Omega_{\Lambda,\eta}$ for the set of all admissible configurations $\sigma \in E^\Lambda$ in Λ which are compatible with some $\eta \in \Omega$, in the sense that the composed configuration $\sigma\eta_{\Lambda^c}$ belongs to Ω. In particular, we write $\Omega_\Lambda = \Omega_{\Lambda,0}$ for the set of all admissible configurations in Λ, which are compatible with the empty configuration 0 outside Λ. It is then easy to see that

$$\mu^{z,q}_{\Lambda,\eta} = \pi^{z,q}_\Lambda(\,\cdot\,|\Omega_{\Lambda,\eta}) \ ,$$

where $\pi^{z,q}_\Lambda = \bigotimes_{i\in\Lambda} \pi^{z,q}_i$ is the Λ-product of the measures $\pi^{z,q}_i = (\frac{1}{1+qz}, \frac{z}{1+qz}, \ldots, \frac{z}{1+qz})$ on E.

Given the Gibbs distributions $\mu^{z,q}_{\Lambda,\eta}$, we define the associated class $\mathcal{G}(z,q)$ of (infinite volume) Gibbs measures on Ω in the usual way [8]. Our main result below shows that for large q there exist two different activity regimes in which $\mathcal{G}(z,q)$ contains several phases of quite different behavior. These regimes meet at a critical activity $z_c(q)$ and produce a first-order phase transition.

The different phases admit a geometric description in percolation terms. Let $\mathbf{Z}^2$ be equipped with the usual graph structure (obtained by drawing edges between sites of Euclidean distance 1). Given any $\sigma \in \Omega$, a subset S of $\mathbf{Z}^2$ will be called an *occupied cluster* if S is a maximal connected subset of $\{i \in \mathbf{Z}^2 : \sigma_i \neq 0\}$, and an *occupied sea* if, in addition, each finite subset Δ of $\mathbf{Z}^2$ is surrounded by a circuit (i.e., closed lattice path) in S. In other words, an occupied sea is an infinite occupied cluster with interspersed finite 'islands'. If in fact $\sigma_i = a$ for all $i \in S$ we say S is an *occupied sea of color a*. We consider also the dual graph structure of $\mathbf{Z}^2$ with so-called $*$edges between sites of distance 1 or $\sqrt{2}$, and the associated concept of $*$connectedness. An *even occupied $*$sea* is a maximal $*$connected subset of $\{i = (i_1, i_2) \in \mathbf{Z}^2 : i_1 + i_2 \text{ even}, \sigma_i \neq 0\}$ containing $*$circuits around arbitrary finite sets Δ. Likewise, an *odd empty $*$sea* is a maximal $*$connected subset of $\{i = (i_1, i_2) \in \mathbf{Z}^2 : i_1 + i_2 \text{ odd}, \sigma_i = 0\}$ surrounding any finite Δ.

Theorem 2.1 *If the number q of colors exceeds some q_0, there exists an activity threshold $z_c(q) \in \,]\,q/5, 5q\,[$ and numbers $0 < \varepsilon(q) < 1/3$ with $\varepsilon(q) \to 0$ as $q \to \infty$ such that the following hold:*

(i) *For $z > z_c(q)$, there exist q distinct translation invariant 'colored' phases $\mu_a \in \mathcal{G}(z,q)$, $a \in \{1, \ldots, q\}$. Relative to μ_a, there exists almost surely an occupied sea of color a containing any given site with probability at least $1 - \varepsilon(q)$.*

(ii) *For $q_0/q \leq z < z_c(q)$, there exist two distinct 'staggered' phases $\mu_{\text{even}}, \mu_{\text{odd}} \in \mathcal{G}(z,q)$ invariant under even translations. Relative to μ_{even}, there exist almost surely both an even occupied $*$sea and an odd empty $*$sea, and any two adjacent sites belong to these $*$seas with probability at least $1 - \varepsilon(q)$. In addition, all occupied clusters are finite almost surely, and their colors are independent and uniformly distributed conditionally on their position. μ_{odd} is obtained from μ_{even} by a one-step translation.*

(iii) *At $z = z_c(q)$, a first-order phase transition occurs, in the sense that $q+2$ distinct phases $\mu_{\rm even}, \mu_{\rm odd}, \mu_1, \ldots, \mu_q \in \mathcal{G}(z_c(q), q)$ coexist which enjoy the properties above.*

The preceding theorem can be summarized by the following phase diagram.

We continue with a series of comments.

Remark 2.1 (1) The existence of staggered phases in an intermediate activity region was first observed by Runnels and Lebowitz [15]. As will become apparent later, this is a consequence of the fact that the lattice $\mathbf{Z}^2$ is bipartite and the interaction is nearest-neighbor. According to Theorem 2.1, for large q the staggered regime extends up to the fully ordered regime, and the transition from the staggered regime to the ordered regime at $z_c(q)$ is of first order. This result (which disproves a conjecture in [15]) has already been obtained before by Lebowitz, Mazel, Nielaba and Šamaj [12]. While their argument relies on Pirogov–Sinai theory (which even gives the asymptotics of $z_c(q)$), we offer here a different proof based on reflection positivity which is quite elementary and can easily be adapted to our other models (including a continuous-spin variant of the present model).

(2) There are two kinds of ordering to be distinguished: positional order and color-order. The colored (or 'demixed') phases $\mu_1, \ldots, \mu_q$ show color-order but no positional order. (The impression of positional order is a delusion coming from the lattice regularity.) Their high density takes advantage of the chemical energy of particles (i.e., of the activity z.) On the other hand, the staggered (or 'crystal') phases $\mu_{\rm even}, \mu_{\rm odd}$ exhibit positional order but color-disorder. Positional *and* color-disorder occurs in the uniqueness regime at sufficiently low activities.

(3) The first-order transition at $z_c(q)$ manifests itself thermodynamically by a jump of the particle density as a function of the activity. In fact, $z_c(q)$ can be characterized as the unique value where the density jumps over the level 2/3, cf. Lemma 3.6.

(4) For small z there exists only one Gibbs measure in $\mathcal{G}(z, q)$. For example, using disagreement percolation one easily finds that this is the case when $qz < p_c/(1 - p_c)$, where p_c is the Bernoulli site percolation threshold for $\mathbf{Z}^2$; see [1, 9] for more details. We do not know whether the uniqueness regime extends right up to the staggered regime. As will be explained in the next comment, this question is related to the behavior of the hard-core lattice gas.

(5) As was already noticed in [15, 12], the occupation structure of the large-q Widom–Rowlinson model at activity z is approximately described by the hard-core lattice gas with activity $\zeta = qz$. This becomes evident from the following argument (which is more explicit than those in [15, 12]). Consider the Gibbs distribution $\mu_{\Lambda,\rm per}$ of our model in a rectangular box Λ with periodic boundary condition. (This boundary condition is natural, since later on we will only look at phases appearing in the extreme decomposition of infinite volume limits of $\mu_{\Lambda,\rm per}$; we could also use empty or monochromatic

boundary conditions instead.) Let $\psi_{\Lambda,\mathrm{per}}$ be the image of $\mu_{\Lambda,\mathrm{per}}$ under the projection $\sigma \to n = (n_i)_{i\in\Lambda} = (1_{\{\sigma_i \neq 0\}})_{i\in\Lambda}$ from E^Λ to $\{0,1\}^\Lambda$ mapping a configuration of colored particles onto the occupation pattern. $\psi_{\Lambda,\mathrm{per}}$ is called the site-random-cluster distribution, see Section 6.7 of [9]. Its conditional probabilities are given by the formula

$$\psi_{\Lambda,\mathrm{per}}(n_i = 1 | n_{\Lambda\setminus\{i\}}) = \frac{qz}{qz + q^{\kappa(i,n)}} \ ,$$

where $\kappa(i,n)$ is the number of clusters of $\{j \in \Lambda \setminus \{i\} : n_j = 1\}$ meeting a neighbor of i. Now, since $\kappa(i,n) = 0$ if and only if all neighbors of i are empty, this conditional probability tends to the one of the hard-core lattice model with activity ζ when $q \to \infty$ and $\zeta = qz$ stays fixed. Unfortunately, this result is *not* sufficient to conclude that in this limit the transition point from the unique to the staggered phase converges to that of the hard-core lattice gas, although this seems likely and is suggested by simulations [12].

(6) One may ask whether the monotonicity of the transition from the staggered to the ordered regime can be deduced from stochastic monotonicity properties of the site-random-cluster model, as is possible in the Potts model. Unlike in the standard (bond) random-cluster model, such a stochastic monotonicity is not available [2]. To obtain the existence of a unique transition point $z_c(q)$ we will therefore use the convexity of the pressure, which implies that the particle density is an increasing function of z.

(7) As is often the case in this kind of context, our bounds on q_0 are not very useful. They only allow us to conclude that we can take e.g. $q_0 = 2 \cdot 10^{85}$. Note that for small q the ordered regime still exists [15], but for $q = 2$ there is no staggered regime but instead a direct second order transition from the gas phase to the ordered phase. For this and more information about the minimal q at which the staggered phase appears see [12, 13].

2.2 The square-shaped Widom–Rowlinson lattice gas

The standard Widom–Rowlinson model considered above is defined by the exclusion rule that no two particles of different color may occupy adjacent sites. Equivalently, one may think of the particles as having the shape of the diamond $\{x \in \mathbf{R}^2 : \|x\|_1 < 1\}$, and diamonds of different color are required to be disjoint.

In this section we want to study a variant with different geometry: we identify a particle at position $i \in \mathbf{Z}^2$ with the suitably colored square $\{x \in \mathbf{R}^2 : \|x - i\|_\infty < 1\}$, and we stipulate that squares of different color are disjoint, while squares of the same color may overlap. Alternatively, this assumption amounts to replacing $\mathbf{Z}^2$ by its matching dual $(\mathbf{Z}^2)^*$, which is obtained from $\mathbf{Z}^2$ by keeping all nearest-neighbor bonds and adding bonds between diagonal neighbors of Euclidean distance $\sqrt{2}$; for lack of a generally accepted name we call this lattice the *face-crossed square lattice*. Accordingly, we say that two sites $i, j \in \mathbf{Z}^2$ are $*$adjacent if $|i - j| = 1$ or $\sqrt{2}$, and we write $\langle ij\rangle^*$ for such pairs of sites. Saying that squares of different colors are disjoint is then equivalent to saying that particles of different color do not sit on $*$adjacent sites.

The point of considering this model is that the square-shape of particles fits better with the geometry of $\mathbf{Z}^2$ than the diamond-shape in the standard Widom–Rowlinson

model. As a consequence, the somehow artificial staggered phases disappear, and the model is closer to what one would expect to hold in the continuum Widom–Rowlinson model.

We now turn to precise statements. The formal Hamiltonian of the square-shaped Widom–Rowlinson model is analogous to (1),

$$H(\sigma) = \sum_{\langle ij \rangle^*} U(\sigma_i, \sigma_j) \ ,$$

with the same pair interaction U as in (2). The variables σ_i still take values in the set $E = \{0, 1, \ldots, q\}$. We then can introduce the same definitions as in Section 2.1, only replacing $\langle ij \rangle$ by $\langle ij \rangle^*$ at all proper places. For simplicity, we refrain from adding $*$'s to the quantities so defined. In particular, we write again $\mathcal{G}(z, q)$ for the set of Gibbs measures in the present square-shaped model.

Given a configuration $\sigma \in \Omega$, we call a subset S of $\mathbf{Z}^2$ an *occupied $*$cluster* if S is a maximal $*$connected subset of $\{i \in \mathbf{Z}^2 : \sigma_i \neq 0\}$. Such an S may be visualized as the connected component in $\mathbf{R}^2$ of the union of all squares with centers in S. We say that two disjoint square-shaped particles are *contiguous* if they touch each other along at least one half of a side (i.e., if their centers have Euclidean distance 2 or $\sqrt{5}$), and are separated by two empty sites. A set S of pairwise disjoint square particles will be called a *contiguity sea* if it is maximal connected relative to the contiguity relation, and the union of their closures surrounds each bounded set.

Our result for this model is the following.

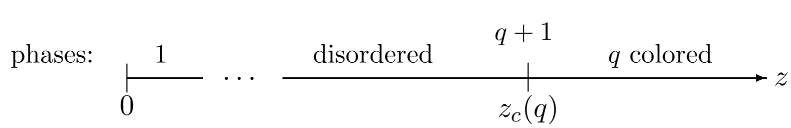
Theorem 2.2 *If q exceeds some sufficiently large q_0, there exist a critical activity $z_c(q) \in \,]\, q^{1/3}/3, 3\, q^{1/3}\, [$ and numbers $0 < \varepsilon(q) < 1/3$ with $\varepsilon(q) \to 0$ as $q \to \infty$ such that the following hold:*

(i) *For $z > z_c(q)$, there exist q distinct translation invariant 'colored' phases $\mu_a \in \mathcal{G}(z, q)$, $a \in \{1, \ldots, q\}$. Relative to μ_a, there exists almost surely an occupied sea of color a containing any given site with probability at least $1 - \varepsilon(q)$.*

(ii) *For $q_0/q \leq z < z_c(q)$, there exists a translation invariant disordered phase $\mu_{\text{dis}} \in \mathcal{G}(z, q)$ such that with probability 1 all occupied $*$clusters are finite, independently and randomly colored, and surrounded by a contiguity sea. Moreover, $\mu_{\text{dis}}(\sigma_i \neq 0) < 1/4 + \varepsilon(q)$ for all i.*

(iii) *At $z = z_c(q)$, a first-order phase transition occurs, in the sense that there exist $q + 1$ distinct phases $\mu_{\text{dis}}, \mu_1, \ldots, \mu_q \in \mathcal{G}(z_c(q), q)$ exhibiting the properties above.*

In short, we have the following phase diagram:



Remark 2.2 (1) The first-order transition at $z_c(q)$ manifests itself thermodynamically by a jump of the particle density from a value close to 1/4 to a value close to 1.

(2) The behavior of the square-shaped Widom–Rowlinson model differs from that of the standard, diamond-shaped Widom–Rowlinson model in that there are no staggered phases but instead only one disordered phase showing not only color-disorder but also positional disorder. In fact, we expect that this disordered phase is the unique Gibbs measure for any $z < z_c(q)$, although this does not follow from our methods. (Just as in Remark 2.1 (5), one can see that for large q the square-shaped Widom–Rowlinson model is related to the square-shaped hard-core lattice gas. It seems that the latter model does not exhibit a phase transition, but we are not aware of any proof.)

(3) The first-order transition at $z_c(q)$ implies a percolation transition from an empty sea in the disordered phase to an occupied sea in the colored phases. In spite of the supposed uniqueness of the Gibbs measure in the whole range $[0, z_c(q)[$, this interval contains a further percolation threshold, namely a critical value for the existence of a contiguity sea. Indeed, for sufficiently small z one can use disagreement percolation [1, 9] to show the uniqueness of the Gibbs measure and the existence of a sea of empty plaquettes; the latter excludes the existence of a contiguity sea. However, it is far from obvious that a contiguity sea will set on at a well-defined activity. This is because neither the existence of a contiguity sea is an increasing event, nor the site-random cluster distributions (which can also be used in the present case) are stochastically monotone in z, cf. Remark 2.1 (6). We note that a similar percolation transition occurs also in the square-shaped hard-core lattice gas [6]; this shows again that the latter describes the limiting behavior of our model in this regime.

2.3 A Widom–Rowlinson model with molecular hard core

Another way of changing the geometry of the Widom–Rowlinson model is to introduce a molecular (i.e., color-independent) hard-core interaction between particles. In this section we will discuss a model variant of this kind.

As before, the underlying lattice is still the square lattice $\mathbf{Z}^2$, and the state space at each lattice site is the set $E = \{0, 1, \ldots, q\}$. The formal Hamiltonian is of the form

$$H(\sigma) = \sum_{|i-j|=1} \Phi(\sigma_i, \sigma_j) + \sum_{|i-j|=\sqrt{2}} U(\sigma_i, \sigma_j) \; ; \tag{4}$$

here Φ, the nearest-neighbor molecular hard-core exclusion, is given by

$$\Phi(\sigma_i, \sigma_j) = \begin{cases} \infty & \text{if } \sigma_i \sigma_j \neq 0 \, , \\ 0 & \text{otherwise,} \end{cases}$$

and the next-nearest neighbor color repulsion U is still defined by (2). The main effect of the molecular hard core is a richer high-density phase diagram containing $2q$ phases with color-order *and* staggered positional order. The low-density regime is disordered both in the sense of color and position, as in the case of the square-shaped Widom–Rowlinson model. The transition between these regimes is still of first order, though the positional order of the high-density phases is an impediment for this to occur. We do not repeat the definitions of admissible configurations and of Gibbs measures, which are straightforward.

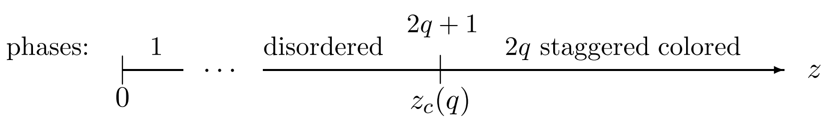
Theorem 2.3 *If $q \geq q_0$ for a suitable q_0, there exist a threshold $z_c(q) \in \,]\, q/18, 18\, q\, [$ and numbers $0 < \varepsilon(q) < 1/5$ with $\varepsilon(q) \to 0$ as $q \to \infty$ such that the following hold:*

(i) *For $z > z_c(q)$ there exist $2q$ distinct colored and staggered phases $\mu_{a,\mathrm{even}}$, $\mu_{a,\mathrm{odd}} \in \mathcal{G}(z, q)$, $a \in \{1, \ldots, q\}$, which are invariant under even translations. Relative to $\mu_{a,\mathrm{even}}$ there exist almost surely both an even occupied $*$sea of color a and an odd empty $*$sea, and any two adjacent sites belong to these $*$seas with probability at least $1 - \varepsilon(q)$. $\mu_{a,\mathrm{odd}}$ is obtained from $\mu_{a,\mathrm{even}}$ by a one-step translation.*

(ii) *For $q_0^{1/7}/q \leq z < z_c(q)$, there exists a translation invariant disordered phase $\mu_{\mathrm{dis}} \in \mathcal{G}(z, q)$ such that with probability 1 all occupied $*$clusters are finite, independently colored with uniform distribution, and enclosed by a contiguity sea. Also, $\mu_{\mathrm{dis}}(\sigma_i \neq 0) < 1/4 + \varepsilon(q)$ for all i.*

(iii) *At $z = z_c(q)$, a first-order phase transition occurs, in the sense that there coexist $2q+1$ distinct phases μ_{dis}, $\mu_{1,\mathrm{even}}$, $\mu_{1,\mathrm{odd}}, \ldots$, $\mu_{q,\mathrm{even}}$, $\mu_{q,\mathrm{odd}} \in \mathcal{G}(z_c(q), q)$, with the properties above.*

We summarize this theorem by the following phase diagram:



Remark 2.3 (1) The first-order transition at $z_c(q)$ manifests itself thermodynamically by a jump of the particle density from a value close to $1/4$ to a value close to $1/2$.

(2) The Widom–Rowlinson model with molecular hard-core may be viewed as a combination of a lattice gas of hard diamonds and the square-shaped Widom–Rowlinson model. Its high-density regime inherits the staggered occupation pattern from the former, and the color order from the latter. The effect of colors is still strong enough to produce a first-order transition, which is absent in the pure hard-diamonds model [12]. Just as in the case of Theorem 2.2, the low density regime is governed by the behavior of the square-shaped hard-core lattice gas. Indeed, it is not difficult to develop a random-cluster representation of the model and to show that its conditional probabilities converge to that of the square-shaped lattice gas when $q \to \infty$ but qz remains fixed; cf. Remark 2.1 (5). Mutatis mutandis, the comments in Remark 2.2 apply here as well.

(3) One may ask what happens if we interchange the rôles of Φ and U in the Hamiltonian of Eq. (4), i.e., if there is a molecular hard core between diagonal neighbors of distance $\sqrt{2}$, and a Widom–Rowlinson intercolor repulsion between nearest particles of distance 1. In this case it is not hard to see that for any $q \geq 2$ and sufficiently large z there exist four different phases with positional order but color disorder. One of these phases (to be called the even vertical phase) has almost surely a sea of sites $i = (i_1, i_2) \in \mathbf{Z}^2$ which are occupied when i_1 is even, and empty when i_1 is odd. The other three phases are obtained by translation and/or interchange of coordinates. However, it seems that in this case the geometry of interaction does not exhibit the properties leading to a first-order transition, so that the transition to the low density regime is of second order. We will return to this point at the end of Section 5.

2.4 A continuous-spin Widom–Rowlinson model

The multitype Widom–Rowlinson lattice model may be viewed as a diluted clock model for which each lattice site is either empty or occupied by a particle with an orientation in the discrete group of q'th roots of unity. This suggests considering the following plane-rotor model of oriented particles which may serve as a simple model of a ferrofluid or liquid crystal.

Consider the state space $E = \{0\} \cup S^1$, equipped with the reference measure $\nu = \delta_0 + \lambda$, where λ is normalized Haar measure on the circle S^1. As before, the equality $\sigma_i = 0$ means that site i is empty, while $\sigma_i = a \in S^1$ says that i is occupied by a particle with orientation a. The formal Hamiltonian is again given by (1), where the pair interaction U is now defined by

$$U(\sigma_i, \sigma_j) = \begin{cases} \infty & \text{if } \sigma_i, \sigma_j \in S^1,\ \sigma_i \cdot \sigma_j \geq \cos 2\pi\alpha\ , \\ 0 & \text{otherwise} \end{cases}$$

for some angle $0 < \alpha < 1/4$. This potential forces adjacent particles to have nearly the same orientation. The parameter α will play the same rôle as $1/q$ did before. The Gibbs distributions $\mu_{\Lambda,\eta}^{z,\alpha}$ in a finite region $\Lambda \subset \mathbf{Z}^2$ with boundary condition η and activity $z > 0$ are defined by their densities with respect to the product measure ν^Λ, which are again given by the right-hand side of equation (3). We write $\mathcal{G}(z, \alpha)$ for the associated set of Gibbs measures. Since U preserves the $O(2)$-symmetry of particle orientations, the Mermin–Wagner–Dobrushin–Shlosman theorem (cf. Theorem (9.20) of [8]) implies that each such Gibbs measure is invariant under simultaneous rotations of particle orientations.

Theorem 2.4 *If α is less than some sufficiently small α_0, there exist a critical activity $z_c(\alpha) \in\,]\,\alpha^{-2}/18, 5\,\alpha^{-2}\,[$ and numbers $0 < \varepsilon(\alpha) < 1/3$ with $\varepsilon(\alpha) \to 0$ as $\alpha \to 0$ such that the following hold:*

(i) *For $z > z_c(\alpha)$ there exists a dense 'ordered' phase $\mu_{\text{ord}} \in \mathcal{G}(z, \alpha)$ exhibiting the translation invariance and $O(2)$-symmetry of the model. Relative to μ_{ord}, there exists almost surely an occupied sea containing any fixed site with probability at least $1 - \varepsilon(\alpha)$ (and on which the orientations of adjacent particles differ only by the angle $2\pi\alpha$).*

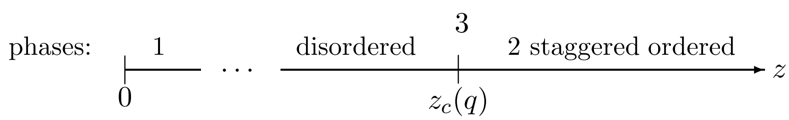
(ii) *For $\alpha_0^{-1} \leq z < z_c(\alpha)$, there exist two distinct 'staggered' phases $\mu_{\text{even}}, \mu_{\text{odd}} \in \mathcal{G}(z, \alpha)$ which are invariant under particle rotations and even translations. Almost surely with respect to μ_{even} there exist both an even occupied $*$sea and an odd empty $*$sea, and any two adjacent sites belong to these $*$seas with probability at least $1 - \varepsilon(q)$. In addition, all occupied clusters are almost surely finite, and conditionally on their position the distribution of orientations is invariant under simultaneous rotations of all spins in a single occupied cluster. μ_{odd} is obtained from μ_{even} by a one-step translation.*

(iii) *At $z = z_c(\alpha)$, a first-order phase transition occurs, in the sense that there exist three distinct phases $\mu_{\text{even}}, \mu_{\text{odd}}, \mu_{\text{ord}} \in \mathcal{G}(z_c(\alpha), q)$ with the properties above.*

The theorem above shows that the present model behaves similarly to the related finite-energy model considered in [4]. Presumably μ_{ord} is the unique Gibbs measure for $z > z_c(\alpha)$, and there is a second-order transition from the staggered regime to the low-activity uniqueness regime. We thus have the following phase diagram.

Remark 2.4 The model above is a continuous-spin counterpart of the standard Widom–Rowlinson model considered in Section 2.1. It is rather straightforward to modify our techniques for investigating analogous continuous-spin variants of the square-shaped Widom–Rowlinson model and of the model with diagonal molecular hard core. In the first case, we obtain a phase diagram of the form

and in the second case we find



The details are left to the reader.

3 Proof of Theorem 2.1

The proof of all four theorems follows the general scheme described in Chapters 18 and 19 of Georgii [8], which is similar in spirit to that of Dobrushin and Shlosman [5] and Kotecký and Shlosman [10]. This scheme consists of two parts: a model-specific contour estimate implying percolation of "good plaquettes", and a general part deducing from this percolation the first-order transition and the properties of phases. We describe the general part first and defer the contour estimate to a second subsection. Many of the details presented here for the Widom–Rowlinson model carry over to the other models, so that for the proofs of Theorems 2.2 to 2.4 we only need to indicate the necessary changes. We note that our arguments can easily be extended to the higher dimensional lattices $\mathbf{Z}^d$ using either the ideas of Chapter 18 of [8] or those of [7].

3.1 Competition of staggered and ordered plaquettes

We consider the standard plaquette $C = \{0,1\}^2$ in $\mathbf{Z}^2$ as well as its translates $C+i$, $i \in \mathbf{Z}^2$. Two plaquettes $C+i$ and $C+j$ will be called adjacent if $|i-j| = 1$, i.e., if $C+i$ and $C+j$ share a side. We are interested in plaquettes with a specified configuration pattern. Each such pattern will be specified by a subset F of Ω_C, the set of admissible configurations in C. For any such F we define a random set $V(F)$ as follows. Let r_1 and r_2 be the reflections of C in the vertical resp. horizontal line in the middle of C, and $r^i = r_1^{i_1} r_2^{i_2}$ the reflection associated to $i = (i_1, i_2) \in \mathbf{Z}^2$. We then let

$$V(F) : \sigma \to \{i \in \mathbf{Z}^2 : r^i \sigma_{C+i} \in F\} \tag{5}$$

be the mapping associating with each $\sigma \in \Omega$ the set of plaquettes on which σ shows the pattern specified by F. (The reflections r^i need to be introduced for reasons of consistency: they guarantee that two adjacent plaquettes may both belong to $V(F)$ even when F is not reflection invariant, as e.g. the sets G_{even} and G_{odd} below.)

We are interested in the case when F is one of the following sets of 'good' configurations on C. These sets are distinguished according to their occupation pattern. Describing a configuration on C by a 2×2 matrix in the obvious way, we define

- $G_{\text{stag}} = G_{\text{even}} \cup G_{\text{odd}} \equiv \{\binom{0\,b}{a\,0} : 1 \le a, b \le q\} \cup \{\binom{a\,0}{0\,b} : 1 \le a, b \le q\}$, the set of all *staggered* configurations with 'diagonal occupations'.
- $G_{\text{ord}} = \bigcup_{1\le a\le q} G_a \equiv \bigcup_{1\le a\le q} \{\binom{a\,a}{a\,a}\}$, the set of all fully *ordered* configurations with four particles of the same color.
- $G = G_{\text{stag}} \cup G_{\text{ord}}$, the set of all good configurations.

Our first objective is to establish percolation of good plaquettes, i.e., of plaquettes in which the configuration is good; the other plaquettes will be called bad. We want to establish this kind of percolation for suitable Gibbs measures *uniformly in the activity* z (provided z is not too small). A suitable class of Gibbs measures is that obtained by infinite-volume limits with periodic boundary conditions.

For any integer $L \ge 1$ we consider the rectangular box

$$\Lambda_L = \{-12\,L + 1, \dots, 12\,L\} \times \{-14\,L + 1, \dots, 14\,L\} \tag{6}$$

in $\mathbf{Z}^2$ of size $v(L) = 24\,L \times 28\,L$. (The reason for this particular choice will become clear in the proofs of Lemmas 3.7 and 3.8.) We write $\mu^{z,q}_{L,\text{per}}$ for the Gibbs distribution in Λ_L with parameters z, q and periodic boundary condition, and $\mathcal{G}_{\text{per}}(z,q)$ for the set of all limiting measures of $\mu^{z,q}_{L,\text{per}}$ as $L \to \infty$ (relative to the weak topology of measures). The basic result is the following *contour estimate* which shows that bad plaquettes have only a small chance to occur.

Proposition 3.1 *For any $\delta > 0$ there exists a number $q_0 \in \mathbf{N}$ such that*

$$\mu(\Delta \cap V(G) = \emptyset) \le \delta^{|\Delta|} \tag{7}$$

whenever $q \ge q_0$, $zq \ge q_0$, $\mu \in \mathcal{G}_{\text{per}}(z,q)$, and $\Delta \subset \mathbf{Z}^2$ is finite.

In the above, $\{\Delta \cap V(G) = \emptyset\}$ is a short-hand for the event consisting of all σ for which all plaquettes $C + i$, $i \in \Delta$, are bad; similar abbreviations will also be used below.

The proof of the proposition takes advantage of reflection positivity and the chessboard estimate, cf. Corollary (17.17) of [8], and is deferred to the next section. We mention here only that q_0 is chosen so large that

$$\delta(q) \equiv q^{-1/56} + q^{-1/12} + q^{-1/4} + q^{-1/2} \le \delta \tag{8}$$

when $q \ge q_0$. It will be essential in the following that the contour estimate is uniform for $z \ge q_0/q$.

As an immediate consequence of the contour estimate we obtain the existence of a *sea of good plaquettes*. We will say that a set of plaquettes forms a sea if the set of their left lower corners is connected and surrounds each finite set. It is then evident that the existence of a sea of completely occupied plaquettes implies the existence of an occupied sea; likewise, the existence of a sea of plaquettes which are occupied on their even points implies the existence of an even occupied $*$sea. In this way, the concept of a sea of plaquettes is general enough to include all concepts of seas introduced in Section 2. Specifically, for any $F \subset \Omega_C$ we define $S(F)$ as the largest sea in $V(F)$ whenever $V(F)$ contains a sea, and let $S(F) = \emptyset$ otherwise.

For $z \geq q_0/q$ we write $\bar{\mathcal{G}}_{\text{per}}(z, q)$ for the set of all accumulation points (in the weak topology) of measures $\mu_n \in \mathcal{G}_{\text{per}}(z_n, q)$ with $z_n \to z$, $z_n \geq q_0/q$. The graph of the correspondence $z \to \bar{\mathcal{G}}_{\text{per}}(z, q)$ is closed; this will be needed in the proof of property (A2) below.

Proposition 3.2 *For any $\varepsilon > 0$ there exists a number $q_0 \in \mathbf{N}$ such that*

$$\mu(0 \in S(G)) \geq 1 - \varepsilon$$

whenever $\mu \in \bar{\mathcal{G}}_{\text{per}}(z, q)$, $q \geq q_0$ and $z \geq q_0/q$.

Proof. Note first that the contour estimate (7) involves only local events and therefore extends immediately to all $\mu \in \bar{\mathcal{G}}_{\text{per}}(z, q)$. The statement then follows directly from Proposition 3.1 together with Lemmas (18.14) and (18.16) of [8]. The number δ has to be chosen so small that $4\delta(1 - 5\delta)^{-2} \leq \varepsilon$. □

What is the advantage of having a sea of good plaquettes? The key property is that the sets G_{stag} and G_{ord} have disjoint side-projections. That is, writing $b = \{(0, 0), (1, 0)\}$ for the two points on the bottom side of C we have

$$\sigma \in G_{\text{stag}}, \sigma' \in G_{\text{ord}} \Rightarrow \sigma_b \neq \sigma'_b ,$$

and similarly for the other sides of C. As a consequence, if two adjacent plaquettes are good then they are both of the same type, either staggered or ordered. Therefore each sea of good plaquettes is either a sea of staggered plaquettes, or a sea of ordered plaquettes. Hence

$$\{S(G) \neq \emptyset\} = \{S(G_{\text{stag}}) \neq \emptyset\} \cup \{S(G_{\text{ord}}) \neq \emptyset\} ,$$

and the two sets on the right-hand side are disjoint. Moreover, the sets G_{even} and G_{odd} also have disjoint side-projections, and so do the sets G_a, $1 \leq a \leq q$. Therefore, the event $\{S(G_{\text{stag}}) \neq \emptyset\}$ splits into the two disjoint subevents $\{S(G_{\text{even}}) \neq \emptyset\}$ and $\{S(G_{\text{odd}}) \neq \emptyset\}$, and $\{S(G_{\text{ord}}) \neq \emptyset\}$ splits off into the disjoint subevents $\{S(G_a) \neq \emptyset\}$, $1 \leq a \leq q$. In other words, each sea of good plaquettes has a characteristic occupation pattern or color corresponding to a particular phase, and we only need to identify the activity regimes for which the different phases do occur.

To this end we fix any $\varepsilon > 0$. We will need later that $\varepsilon < 1/6$. As in the proof of Proposition 3.2, we choose some $0 < \delta < 1/25$ such that $4\delta(1 - 5\delta)^{-2} \leq \varepsilon$, and we let

q_0 be so large that condition (8) holds for all $q \geq q_0$. For such q_0 and q we consider the two activity domains

$$A_{\text{stag}} = \Big\{ z \geq q_0/q : \mu(0 \in V(G_{\text{stag}})) \geq \mu(0 \in V(G_{\text{ord}})) \text{ for some } \mu \in \bar{\mathcal{G}}_{\text{per}}(z,q) \Big\}$$

and

$$A_{\text{ord}} = \Big\{ z \geq q_0/q : \mu(0 \in V(G_{\text{ord}})) \geq \mu(0 \in V(G_{\text{stag}})) \text{ for some } \mu \in \bar{\mathcal{G}}_{\text{per}}(z,q) \Big\} .$$

Our next result shows that these sets describe the regimes in which staggered resp. ordered phases exist. The *mean particle density* $\varrho(\mu)$ of a measure μ which is periodic under translations with period 2 is defined by

$$\varrho(\mu) = \mu(N_C)/|C| \, ; \tag{9}$$

recall that N_C is the number of particles in C.

Proposition 3.3 (a) *For each $z \in A_{\text{stag}}$ there exist two 'staggered' Gibbs measures $\mu_{\text{even}}, \mu_{\text{odd}} \in \mathcal{G}(z,q)$ invariant under even translations of $\mathbf{Z}^2$ and permutations of particle colors. μ_{even}-almost surely we have $S(G_{\text{even}}) \neq \emptyset$, and all occupied clusters are finite and have independently distributed random colors. In addition, $\mu_{\text{even}}(0 \in S(G_{\text{even}})) \geq 1-2\varepsilon$, and in particular $\varrho(\mu_{\text{even}}) \leq \frac{1}{2} + \varepsilon$. μ_{odd} has the analogous properties.*

(b) *For each $z \in A_{\text{ord}}$ there exist q 'colored' translation invariant Gibbs measures $\mu_a \in \mathcal{G}(z,q)$, $a \in \{1,\dots,q\}$. Each μ_a satisfies $\mu_a(S(G_a) \neq \emptyset) = 1$, $\mu_a(0 \in S(G_a)) \geq 1-2\varepsilon$, and in particular has mean particle density $\varrho(\mu_a) \geq 1-2\varepsilon$.*

Proof. (a) Let $z \in A_{\text{stag}}$ be given and $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ be such that $\mu(0 \in V(G_{\text{stag}})) \geq \mu(0 \in V(G_{\text{ord}}))$. Then $\mu(0 \in V(G_{\text{ord}})) \leq 1/2$ and therefore

$$\begin{aligned} \mu\Big(0 \in S(G_{\text{stag}})\Big) &= \mu\Big(0 \in S(G),\, 0 \notin V(G_{\text{ord}})\Big) \\ &\geq 1 - \varepsilon - \frac{1}{2} = \frac{1}{2} - \varepsilon > 0 \, . \end{aligned}$$

But G_{stag} splits into the two parts G_{even} and G_{odd} which are related to each other by the reflection in the line $\{x_1 = 1/2\}$, and μ is invariant under this reflection. Hence

$$p \equiv \mu\Big(0 \in S(G_{\text{even}})\Big) = \mu\Big(0 \in S(G_{\text{odd}})\Big) \geq \frac{1}{2}\left(\frac{1}{2} - \varepsilon\right) > 0 \, .$$

We can therefore define the conditional probabilities $\mu_{\text{even}} = \mu(\,\cdot\,|S(G_{\text{even}}) \neq \emptyset)$ and $\mu_{\text{odd}} = \mu(\,\cdot\,|S(G_{\text{odd}}) \neq \emptyset)$. Since the events in the conditions are tail measurable, these measures belong to $\mathcal{G}(z,q)$. It is clear that these conditional probabilities inherit all common invariance properties of μ and the conditioning events. Moreover, we find

$$\begin{aligned} \mu\Big(S(G_{\text{even}}) \neq \emptyset\Big) &= \frac{1}{2}\,\mu\Big(S(G_{\text{stag}}) \neq \emptyset\Big) \\ &\leq \frac{1}{2}\,\mu\Big(0 \in S(G_{\text{stag}})\Big) + \frac{1}{2}\,\mu\Big(0 \notin S(G)\Big) \\ &\leq p + \frac{\varepsilon}{2} \, , \end{aligned}$$

and therefore

$$\mu_{\text{even}}\Big(0 \in S(G_{\text{even}})\Big) \geq \frac{p}{p+\varepsilon/2} \geq 1-2\varepsilon \ .$$

In particular, it follows that

$$\varrho(\mu_{\text{even}}) \leq \frac{1}{2}\,\mu_{\text{even}}\Big(0 \in V(G_{\text{even}})\Big) + \mu_{\text{even}}\Big(0 \notin V(G_{\text{even}})\Big) \leq \frac{1}{2} + \varepsilon \ .$$

Finally, we show that μ_{even}-almost surely all occupied clusters are finite, and their colors are conditionally independent and uniformly distributed when all particle positions are fixed. Indeed, since $\mu_{\text{even}}(S(G_{\text{even}}) \neq \emptyset) = 1$ there exists μ_{even}-almost surely an odd empty $*$sea. This means that any box Δ is almost surely surrounded by an empty $*$circuit. On the one hand, this shows that all occupied clusters must be finite almost surely. On the other hand, for any $\eta > 0$ we can find a box $\Delta' \supset \Delta$ containing an empty $*$circuit around Δ with probability at least $1-\eta$. Let Γ be the largest set with $\Delta \subset \Gamma \subset \Delta'$ such that there are no particles on its outer boundary $\partial\Gamma$; if no such set exists we set $\Gamma = \emptyset$. The events $\{\Gamma = \Lambda\}$ then depend only on the configuration in $\mathbf{Z}^2\setminus\Lambda$. By the strong Markov property of μ_{even}, we conclude that on $\{\Gamma \neq \emptyset\}$ the distribution of colors of the occupied clusters meeting Δ is governed by the Gibbs distribution in Γ with empty boundary condition. The symmetry properties of the latter thus imply that these colors are conditionally independent and uniformly distributed. Letting $\eta \to 0$ and $\Delta \uparrow \mathbf{Z}^2$ we find that this statement holds in fact for all occupied clusters.

By construction, μ_{odd} is obtained from μ_{even} by a one-step translation, and thus has the analogous properties.

(b) The proof of this part is quite similar. Pick any $z \in A_{\text{ord}}$ and $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ such that $\mu(0 \in V(G_{\text{ord}})|0 \in V(G)) \geq 1/2$. Since μ is invariant under permutations of colors it then follows in the same way that

$$p \equiv \mu\Big(0 \in S(G_a)\Big) \geq \frac{1}{q}\left(\frac{1}{2} - \varepsilon\right) > 0 \ ,$$

so that we can define the conditional probabilities $\mu_a = \mu(\,\cdot\,|S(G_a) \neq \emptyset) \in \mathcal{G}(z,q)$, $a \in \{1,\ldots,q\}$. Also,

$$\mu\Big(S(G_a) \neq \emptyset\Big) \leq \frac{1}{q}\,\mu\Big(0 \in S(G_{\text{ord}})\Big) + \frac{1}{q}\,\mu\Big(0 \notin S(G)\Big) \leq p + \frac{\varepsilon}{q} \ ,$$

whence $\mu_a(0 \in S(G_a)) \geq p/(p+\varepsilon/q) \geq 1-2\varepsilon$ and $\varrho(\mu_a) \geq \mu_a(0 \in V(G_a)) \geq 1-2\varepsilon$. □

According to the preceding proposition, Theorem 2.1 will be proved once we have shown that there exists a critical activity $z_c(q) \in \,]\,q/5, 5q\,[$ such that $A_{\text{stag}} = [q_0/q, z_c(q)]$ and $A_{\text{ord}} = [z_c(q), \infty[$. To this end we will establish the following items:

(A1) $A_{\text{stag}} \cup A_{\text{ord}} = [q_0/q, \infty[$.

(A2) A_{stag} and A_{ord} are closed.

(A3) $A_{\text{ord}} \cap [q_0/q, q/5] = \emptyset$.

(A4) $A_{\text{stag}} \cap [5q, \infty[= \emptyset$.

(A5) $|A_{\text{stag}} \cap A_{\text{ord}}| \leq 1$.

Statement (A1) follows trivially from the definitions of A_{stag} and A_{ord}. Assertion (A2) is also obvious because these definitions involve only local events, and the graph of the correspondence $z \to \bar{\mathcal{G}}_{\text{per}}(z,q)$ is closed by definition.

Property (A3) corresponds to the discovery of Runnels and Lebowitz [15] that staggered phases do exist in a nontrivial activity regime, and follows directly from the next result.

Lemma 3.4 *For $z \leq q/5$ and $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ we have*

$$\mu\Big(0 \in V(G_{\text{ord}}) \Big| 0 \in V(G)\Big) < 1/2 \ .$$

Proof. Consider the Gibbs distribution $\mu^{z,q}_{L,\text{per}}$ in the box Λ_L with periodic boundary condition, and let

$$G_{\text{ord},L} = \Big\{\sigma \in \Omega_{L,\text{per}} : \sigma_{C(i)} \in G_{\text{ord}} \text{ for all } i \in \Lambda_L\Big\}\,; \tag{10}$$

here we write $\Omega_{L,\text{per}}$ for the set of admissible configurations in the torus Λ_L (including nearest-neighbor bonds between the left and the right sides as well as between the top and bottom sides of Λ_L), and $C(i)$ for the image $C+i \bmod \Lambda_L$ of C under the periodic shift of Λ_L by i. (As G_{ord} is reflection-symmetric, we can omit the reflections r^i which appear in (5).) The chessboard estimate (cf. Corollary (17.17) of [8]) then implies that

$$\mu^{z,q}_{L,\text{per}}\Big(0 \in V(G_{\text{ord}})\Big) \leq \mu^{z,q}_{L,\text{per}}(G_{\text{ord},L})^{1/v(L)} \ .$$

We compare the latter probability with that of the event

$$G_{\text{even},L} = \Big\{\sigma \in \Omega_{L,\text{per}} : r^i\sigma_{C(i)} \in G_{\text{even}} \text{ for all } i \in \Lambda_L\Big\} \ . \tag{11}$$

This gives

$$\mu^{z,q}_{L,\text{per}}(G_{\text{ord},L}) \leq \mu^{z,q}_{L,\text{per}}(G_{\text{ord},L})\Big/\mu^{z,q}_{L,\text{per}}(G_{\text{even},L}) = z^{v(L)}q\ z^{-v(L)/2}q^{-v(L)/2}$$

because $G_{\text{ord},L}$ contains only the q distinct close packed monochromatic configurations, while for $\sigma \in G_{\text{even},L}$ the $v(L)/2$ particles can have independent colors. Taking the $v(L)$'th root and letting $L \to \infty$ we find for $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$

$$\mu\Big(0 \in V(G_{\text{ord}})\Big) \leq (z/q)^{1/2} \leq 5^{-1/2} < (1-\delta)/2 \ .$$

The last inequality comes from the choice of δ. Since $\mu(0 \in V(G)) \geq 1-\delta$ by Proposition 3.1, the lemma follows. □

Assertion (A4) corresponds to the well-known fact that q ordered phases exist when the activity is large. For $q=2$ this was already shown by Lebowitz and Gallavotti [11], and for arbitrary q by Runnels and Lebowitz [15]. This is again a simple application of the chessboard estimate.

Lemma 3.5 *For $z \geq 5q$ and $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ we have*

$$\mu\Big(0 \in V(G_{\text{stag}}) \Big| 0 \in V(G)\Big) < 1/2 \ .$$

Proof. Let $G_{\mathrm{ord},L}$ be as in (10), and define $G_{\mathrm{stag},L}$ analogously. By the chessboard estimate we find

$$\begin{aligned} \mu^{z,q}_{L,\mathrm{per}}\Big(0 \in V(G_{\mathrm{stag}})\Big) &\leq \mu^{z,q}_{L,\mathrm{per}}(G_{\mathrm{stag},L})^{1/v(L)} \\ &\leq \Big(\mu^{z,q}_{L,\mathrm{per}}(G_{\mathrm{stag},L})\Big/\mu^{z,q}_{L,\mathrm{per}}(G_{\mathrm{ord},L})\Big)^{1/v(L)} \\ &\leq 2^{1/v(L)} z^{1/2} q^{1/2}\, z^{-1} q^{-1/v(L)} \end{aligned}$$

because $G_{\mathrm{stag},L} = G_{\mathrm{even},L} \cup G_{\mathrm{odd},L}$ contains $2\,q^{v(L)/2}$ distinct configurations of particle density 1/2. We can now complete the argument as in the preceding proof. □

For the proof of (A5) we will use a thermodynamic argument, namely the convexity of the pressure as a function of $\log z$. For any translation invariant probability measure μ on Ω we consider the *entropy per volume*

$$s(\mu) = \lim_{|\Lambda|\to\infty} |\Lambda|^{-1}\, S(\mu_\Lambda)\ .$$

Here we write μ_Λ for the restriction of μ to Ω_Λ,

$$S(\mu_\Lambda) = -\sum_{\sigma\in\Omega_\Lambda} \mu_\Lambda(\sigma)\, \log \mu_\Lambda(\sigma)$$

is the entropy of μ_Λ, and the notation $|\Lambda| \to \infty$ means that Λ runs through a specified increasing sequence of square boxes; for the existence of $s(\mu)$ we refer to [8, 14].

We define the thermodynamic *pressure* by

$$P(\log z) = \max_{\mu} \Big[\varrho(\mu)\, \log z + s(\mu)\Big]\ ; \tag{12}$$

the maximum extends over all translation invariant probability measures μ on Ω, and $\varrho(\mu) = \mu(\sigma_0 \neq 0)$ is the associated mean particle density, cf. (9). (Since Ω is defined as the set of all admissible configurations, the hard-core intercolor repulsion is taken into account automatically.) By definition, P is a convex function of $\log z$, and the variational principle (see Theorems 4.2 and 3.12 of [14]) asserts that the maximum in (12) is attained precisely on $\mathcal{G}_\Theta(z,q)$, the set of all translation invariaion invariant elements of $\mathcal{G}(z,q)$. By standard arguments (cf. Remark (16.6) and Corollary (16.15) of [8]) it follows that P is strictly convex, and

$$P'_-(\log z) \leq \varrho(\mu) \leq P'_+(\log z) \text{ for all } \mu \in \mathcal{G}_\Theta(z,q)\ ; \tag{13}$$

here we write P'_- and P'_+ for the left-hand resp. right-hand derivative of P. By strict convexity, P'_- and P'_+ are strictly increasing and almost everywhere identical. Assertion (A5) thus follows from the lemma below.

Lemma 3.6 *For each $z \in A_{\mathrm{stag}} \cap A_{\mathrm{ord}}$ we have $P'_-(\log z) \leq 2/3 \leq P'_+(\log z)$.*

Proof. This has already been shown essentially in Proposition 3.3. Pick any $z \in A_{\mathrm{stag}} \cap A_{\mathrm{ord}}$, and let $\mu \in \bar{\mathcal{G}}_{\mathrm{per}}(z,q)$ be as in the proof of Proposition 3.3(a). Consider the conditional probability $\mu_{\mathrm{stag}} = \mu(\,\cdot\,|S(G_{\mathrm{stag}}) \neq \emptyset) = \frac{1}{2}\,\mu_{\mathrm{even}} + \frac{1}{2}\,\mu_{\mathrm{odd}}$. By the arguments

there, μ_{stag} is well-defined, belongs to $\mathcal{G}_\Theta(z,q)$, and satisfies $\varrho(\mu_{\text{stag}}) \leq 1/2+\varepsilon < 2/3$. On the other hand, the measures μ_a constructed in Proposition 3.3(b) also belong to $\mathcal{G}_\Theta(z,q)$ and satisfy $\varrho(\mu_a) \geq 1-2\varepsilon > 2/3$. The lemma thus follows from (13). □

We can now complete the proof of Theorem 2.1. Properties (A1) to (A4) together imply that $A_{\text{stag}} \cap A_{\text{ord}} \neq \emptyset$. This is because the interval $[q_0/q, \infty[$ is connected and therefore cannot be the union of two disjoint non-empty closed sets. Combining this with (A5) we find that $A_{\text{stag}} \cap A_{\text{ord}}$ consists of a unique value $z_c(q)$. In particular, A_{ord} cannot contain any value $z < z_c(q)$ because the infimum of such z's would belong to $A_{\text{stag}} \cap A_{\text{ord}}$; likewise, A_{stag} does not contain any value $z > z_c(q)$. Hence $A_{\text{stag}} = [q_0/q, z_c(q)]$ and $A_{\text{ord}} = [z_c(q), \infty[$, and Theorem 2.1 follows from Proposition 3.3.

3.2 Contour estimates

In this subsection we will prove Proposition 3.1. Consider the set Ω_C of all admissible configurations in C, and the set $B = \Omega_C \setminus G$ of all bad configurations in C. We split B into the following subsets which are distinguished by their occupation pattern:

- $B_0 = \{\binom{0\,0}{0\,0}\}$, the singleton consisting of the empty configuration in C.
- $B_1 = \{\binom{0\,0}{a\,0}, \binom{0\,0}{0\,a}, \binom{0\,a}{0\,0}, \binom{a\,0}{0\,0} : 1 \leq a \leq q\}$, the set of all configurations with a single particle in C.
- $B_2 = \{\binom{a\,a}{0\,0}, \binom{a\,0}{a\,0}, \binom{0\,0}{a\,a}, \binom{0\,a}{0\,a} : 1 \leq a \leq q\}$, the set of admissible configurations for which one side of C is occupied, and the other side is empty.
- $B_3 = \{\binom{a\,a}{0\,a}, \binom{a\,a}{a\,0}\}, \binom{a\,0}{a\,a}, \binom{0\,a}{a\,a} : 1 \leq a \leq q\}$, the set of all admissible configurations with three particles in C.

We then clearly have $B = \bigcup_{k=0}^{3} B_k$. The four different kinds of "badness" of a plaquette will be treated separately in the three lemmas below. We start with the most interesting case of plaquettes with three particles.

For any $L \geq 1$ and $k \in \{0, \ldots, 3\}$ let

$$B_{k,L} = \{\sigma \in \Omega_{L,\text{per}} : \sigma_{C(i)} \in B_k \text{ for all } i \in \Lambda_L\} ,$$

where $C(i)$ is as in (10). Consider the quantities $p_{k,L}^{z,q} = \mu_{L,\text{per}}^{z,q}(B_{k,L})^{1/v(L)}$ and $p_k^{z,q} = \limsup_{L\to\infty} p_{k,L}^{z,q}$.

Lemma 3.7 $p_3^{z,q} \leq q^{-1/56}$ *for all* $z > 0$ *and* $q \in \mathbf{N}$.

Proof. Fix any integer $L \geq 1$ and consider the set $B_{3,L}$ of configurations σ in Λ_L having a single empty site in each plaquette. We claim that $|B_{3,L}| < q\, 2^{14L+2}$. First of all, for each $\sigma \in B_{3,L}$ the occupied sites in Λ_L form a connected set, so that all particles have the same color. Thus there are only q possible colorings, and we only need to count the possible occupation patterns for $\sigma \in B_{3,L}$. It is easy to see that the plaquettes $C(i)$ with $\sigma(i) = 0$ form a partition of Λ_L. For each such partition, the plaquettes are either arranged in rows or in columns. In the first case, each row is determined by

its parity (even or odd), namely the parity of i_1 for each $C(i)$ in this row; likewise, in the second case each column is determined by its parity. We can therefore count all such partitions as follows. There are 4 possibilities of choosing the plaquette containing the origin. If this plaquette is fixed, there are no more than 2^{14L-1} possibilities of arranging all plaquettes in rows and choosing the parity of each row. Similarly, there are at most 2^{12L-1} possibilities of arranging the plaquettes in columns. The number of such partitions is therefore no larger than $4(2^{14L-1}+2^{12L-1})$, and the claim follows.

To estimate $\mu^{z,q}_{L,\mathrm{per}}(B_{3,L})$ we will rearrange the positions of all particles so that many different colors become possible. More precisely, we divide Λ_L into $(3L)(4L)$ rectangular cells $\Delta(j)$ of size 8×7. Let $\Delta_0(j)$ be the rectangular cell of size 7×6 situated in the left lower corner of $\Delta(j)$, and consider the set

$$F_{3,L}=\{\sigma\in\Omega_{L,\mathrm{per}}:\sigma\neq 0 \text{ on } \Delta_0(j),\ \sigma\equiv 0 \text{ on } \Delta(j)\setminus\Delta_0(j) \text{ for all } j\}\ .$$

Since $|\Delta(j)\setminus\Delta_0(j)|=8\cdot 7-7\cdot 6=|\Delta(j)|/4$ for all j, each $\sigma\in F_{3,L}$ has particle number $3\,v(L)/4$, just as the configurations in $B_{3,L}$. As the colors of the particles in the blocks $\Delta_0(j)$ can be chosen independently, we have $|F_{3,L}|=q^{12L^2}=q^{v(L)/56}$. (The above construction, together with a similar construction in the proof of the next lemma, explains our choice of the rectangle Λ_L.) Now we can write

$$\mu^{z,q}_{L,\mathrm{per}}(B_{3,L})\leq\frac{\mu^{z,q}_{L,\mathrm{per}}(B_{3,L})}{\mu^{z,q}_{L,\mathrm{per}}(F_{3,L})}=\frac{|B_{3,L}|}{|F_{3,L}|}\leq 2^{14L+2}\,q^{1-v(L)/56}\ .$$

The proof is completed by taking the $v(L)$'th root and letting $L\to\infty$. $\square$

Next we estimate the probability of plaquettes with two adjacent particles at one side of C.

Lemma 3.8 *$p^{z,q}_2\leq q^{-1/12}$ for all $z>0$ and $q\in\mathbf{N}$.*

Proof. Fix any $L\geq 1$, and let $\sigma\in B_{2,L}$. Then the particles are either arranged in alternating occupied and empty rows, or in alternating occupied and empty columns. The colors in all rows resp. columns can be chosen independently of each other. Hence $|B_{2,L}|=2(q^{14L}+q^{12L})\leq 4\,q^{14L}$. Moreover, each $\sigma\in B_{2,L}$ has particle number $v(L)/2$. As in the last proof, we construct a set $F_{2,L}$ of configurations with the same particle number but larger color entropy as follows.

We partition Λ_L into $(8L)(7L)$ rectangular cells $\Delta(j)$ of size 3×4, and let $\Delta_0(j)$ be the rectangular cell of size 2×3 in the left lower corner of $\Delta(j)$. We then define

$$F_{2,L}=\{\sigma\in\Omega_{L,\mathrm{per}}:\sigma\neq 0 \text{ on } \Delta_0(j),\ \sigma\equiv 0 \text{ on } \Delta(j)\setminus\Delta_0(j) \text{ for all } j\}\ .$$

Since $|\Delta(j)\setminus\Delta_0(j)|=3\cdot 4-2\cdot 3=|\Delta(j)|/2$ for all j, each $\sigma\in F_{2,L}$ has particle number $v(L)/2$. As the particle colors in the blocks $\Delta_0(j)$ can be chosen independently, we have $|F_{3,L}|=q^{56\,L^2}=q^{v(L)/12}$. As in the last proof, we thus find

$$\mu^{z,q}_{L,\mathrm{per}}(B_{2,L})\leq\frac{\mu^{z,q}_{L,\mathrm{per}}(B_{2,L})}{\mu^{z,q}_{L,\mathrm{per}}(F_{2,L})}=\frac{|B_{2,L}|}{|F_{2,L}|}\leq 4\,q^{14L-v(L)/12}\ .$$

Taking the $v(L)$'th root and letting $L \to \infty$ we obtain the result. $\square$

Finally we consider the probability of 'diluted' plaquettes with a single or no particle.

Lemma 3.9 $p_0^{z,q} \le (zq)^{-1/2}$ *and* $p_1^{z,q} \le (zq)^{-1/4}$ *for all* $z > 0$, $q \in \mathbf{N}$.

Proof. We consider first the case of no particle. For each $L \ge 1$ we can write

$$\mu_{L,\text{per}}^{z,q}(B_{0,L}) \le \frac{\mu_{L,\text{per}}^{z,q}(B_{0,L})}{\mu_{L,\text{per}}^{z,q}(G_{\text{even},L})} = \frac{1}{z^{v(L)/2} q^{v(L)/2}} \ ,$$

where $G_{\text{even},L}$ is defined by (11). The identity follows from the facts that $B_{0,L}$ contains only the empty configuration, whereas each configuration in $G_{\text{even},L}$ consists of $v(L)/2$ particles with arbitrary colors. The first result is thus obvious.

Turning to the case of a single particle per plaquette, we note that each $\sigma \in B_{1,L}$ consists of $v(L)/4$ particles with arbitrary colors, and there are no more than 2^{14L+2} distinct occupation patterns for these particles; the latter follows as in the proof of Lemma 3.7 (by interchanging empty and occupied sites). Hence

$$\mu_{L,\text{per}}^{z,q}(B_{1,L}) \le \frac{\mu_{L,\text{per}}^{z,q}(B_{1,L})}{\mu_{L,\text{per}}^{z,q}(G_{\text{even},L})} \le \frac{2^{14L+2} z^{v(L)/4} q^{v(L)/4}}{z^{v(L)/2} q^{v(L)/2}} \ ,$$

and the second result follows by taking the $v(L)$'th root and letting $L \to \infty$. $\square$

Proof of Proposition 3.1. Let $\mu \in \mathcal{G}_{\text{per}}(z,q)$ and a finite $\Delta \subset \mathbf{Z}^2$ be given. Then we can write

$$\begin{aligned}
\mu(\Delta \cap V(G) = \emptyset) &= \sum_{\gamma:\Delta \to \{0,\dots,3\}} \mu(\sigma : \sigma_{C+i} \in B_{\gamma(i)} \text{ for all } i \in \Delta) \\
&\le \sum_{\gamma:\Delta \to \{0,\dots,3\}} \limsup_{L\to\infty} \mu_{L,\text{per}}^{z,q}(\sigma : \sigma_{C(i)} \in B_{\gamma(i)} \text{ for all } i \in \Delta) \\
&\le \sum_{\gamma:\Delta \to \{0,\dots,3\}} \limsup_{L\to\infty} \prod_{i\in\Delta} p_{\gamma(i),L}^{z,q} \\
&\le \Big(\sum_{k=0}^{3} p_k^{z,q}\Big)^{|\Delta|} .
\end{aligned}$$

In the third step we have used the chessboard estimate, see Corollary (17.17) of [8]. Inserting the estimates of Lemmas 3.7, 3.8 and 3.9 and choosing q_0 as in (8) we get the result. $\square$

4 Proof of Theorem 2.2

Here we indicate how the proof of Theorem 2.1 can be adapted to obtain Theorem 2.2. First of all, the different geometry of the present model leads to a new classification of good and bad plaquettes: the ordered configurations in G_{ord} are still good, but the (former good) configurations in G_{stag} are now bad and will be denoted by B_{stag}, while the configurations in B_1 are now good, and we set $G_{\text{dis}} = B_1$.

We first need an analog of the contour estimate, Proposition 3.1. Remarkably, the estimates of Lemmas 3.7 and 3.8 carry over without any change. To deal with B_{stag} we can proceed exactly as in Lemma 3.8, noting that each configuration in $B_{\text{stag},L}$ is monochromatic, so that $|B_{\text{stag},L}| = 2\,q$. This shows that also $p_{\text{stag}}^{z,q} \le q^{-1/12}$. Finally, for B_0 we compare the set $B_{0,L}$ with

$$F_{1,L} = \{\sigma \in \Omega_{L,\text{per}} : \sigma_i \neq 0 \text{ iff } i \in 2\,\mathbf{Z}^2\}\ ; \tag{14}$$

this gives $p_0^{z,q} \le (zq)^{-1/4}$. The counterpart of Proposition 3.1 thus holds as soon as q_0 is so large that $q_0^{-1/56} + 2\,q_0^{-1/12} + q_0^{-1/4} \le \delta$.

With the contour estimate in hand we can then proceed as in Section 3.1. Proposition 3.3 carries over verbatim; the only difference is that G_{stag} is replaced by G_{dis} (which is not divided into two parts with disjoint side-projections), and $\varrho(\mu_{\text{dis}}) \le \frac{1}{4}(1-2\varepsilon)+2\varepsilon = \frac{1}{4}+\frac{3\varepsilon}{2}$. By the latter estimate, the assumption $\varepsilon < 1/6$ is slightly stronger than necessary for adapting Lemma 3.6 to the present case, but we stick to it for simplicity.

The counterparts of Lemmas 3.4 and 3.5 are obtained as follows. On the one hand, we have the estimate

$$\mu_{L,\text{per}}^{z,q}(G_{\text{ord},L}) \le \mu_{L,\text{per}}^{z,q}(G_{\text{ord},L}) \Big/ \mu_{L,\text{per}}^{z,q}(F_{1,L}) \le z^{v(L)} q\; z^{-v(L)/4} q^{-v(L)/4}\ ,$$

showing that

$$\mu\Big(0 \in V(G_{\text{ord}})\Big) \le (z^3/q)^{1/4} \le 3^{-3/4} < (1-\delta)/2$$

when $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ and $z \le q^{1/3}/3$. On the other hand, as in Lemma 3.9 we find

$$\mu_{L,\text{per}}^{z,q}(G_{\text{dis},L}) \le \mu_{L,\text{per}}^{z,q}(G_{\text{dis},L}) \Big/ \mu_{L,\text{per}}^{z,q}(G_{\text{ord},L}) \le \frac{2^{14L+2} z^{v(L)/4} q^{v(L)/4}}{z^{v(L)} q}$$

and therefore

$$\mu\Big(0 \in V(G_{\text{dis}})\Big) \le (q/z^3)^{1/4} \le 3^{-3/4} < (1-\delta)/2$$

when $\mu \in \bar{\mathcal{G}}_{\text{per}}(z,q)$ and $z \ge 3\,q^{1/3}$. With these ingredients it is now straightforward to complete the proof of Theorem 2.2 along the lines of Section 3.1 .

5 Proof of Theorem 2.3

Here we consider the Widom–Rowlinson model with molecular hard-core exclusion. We look again at good configurations in plaquettes. The set Ω_C of admissible configurations in C splits into the good sets

$$G_{\text{ord}} = G_{\text{even}} \cup G_{\text{odd}} = \bigcup_{1\le a\le q} G_{a,\text{even}} \cup G_{a,\text{odd}} \equiv \bigcup_{1\le a\le q} \{\left(\begin{smallmatrix}0 & a\\ a & 0\end{smallmatrix}\right)\} \cup \{\left(\begin{smallmatrix}a & 0\\ 0 & a\end{smallmatrix}\right)\}$$

of *ordered staggered* configurations, the good set

$$G_{\text{dis}} = B_1 = \{\left(\begin{smallmatrix}0 & 0\\ a & 0\end{smallmatrix}\right), \left(\begin{smallmatrix}0 & 0\\ 0 & a\end{smallmatrix}\right), \left(\begin{smallmatrix}0 & a\\ 0 & 0\end{smallmatrix}\right), \left(\begin{smallmatrix}a & 0\\ 0 & 0\end{smallmatrix}\right) : 1 \le a \le q\}$$

of *disordered* configurations, and the only bad set B_0 consisting of the empty configuration. The main technical problem which is new in the present model is that the

sets $G_{\rm ord}$ and $G_{\rm dis}$ *fail* to have disjoint side-projections (although this is the case for the sets $G_{a,\rm even}$ and $G_{a,\rm odd}$). We therefore cannot simply consider sets of good plaquettes, but need to consider the sets of "good plaquettes with neighbors in the same phase". Accordingly, we introduce the random sets

$$\begin{aligned}\hat V(G_{\rm ord}) &= \{i \in V(G_{\rm ord}) : i + (1,0), i + (0,1) \in V(G_{\rm ord})\} \ ,\\ \hat V(G_{\rm dis}) &= \{i \in V(G_{\rm dis}) : i + (1,0), i + (0,1) \in V(G_{\rm dis})\} \ ,\end{aligned}$$

and $\hat V(G) = \hat V(G_{\rm ord}) \cup \hat V(G_{\rm dis})$. By definition, a sea in $\hat V(G)$ then contains either a sea in $\hat V(G_{\rm ord})$ or a sea in $\hat V(G_{\rm dis})$. To establish the existence of such a sea we use the following contour estimate.

Proposition 5.1 *For any $\delta > 0$ there exists a number $q_0 \in \mathbf{N}$ such that*

$$\mu(\Delta \cap \hat V(G) = \emptyset) \le \delta^{|\Delta|}$$

whenever $q \ge q_0$, $zq \ge q_0^{1/7}$, $\mu \in \mathcal{G}_{\rm per}(z,q)$, and $\Delta \subset \mathbf{Z}^2$ is finite.

Proof. Let us start by introducing some notations. We consider the sublattices

$$\mathcal{L}_{1,\rm even} = \{i = (i_1,i_2) \in \mathbf{Z}^2 : i_1 \text{ is even}\} \ , \quad \mathcal{L}_{1,\rm odd} = \mathbf{Z}^2 \setminus \mathcal{L}_{1,\rm even} \ ,$$

and their rotation images $\mathcal{L}_{2,\rm even}$ and $\mathcal{L}_{2,\rm odd}$ which are similarly defined. We also introduce the horizontal double-plaquette

$$D_1 = C \cup (C + (1,0)) = \{0,1,2\} \times \{0,1\}$$

and the event

$$E_1 = \Big\{\sigma \in E^{D_1} : \sigma_C \in G_{\rm ord},\ \sigma_{C+(1,0)} \in G_{\rm dis},\ \text{or vice versa}\Big\}$$

that the two sub-plaquettes of D_1 are good but of different type. E_1 thus consists of the configurations of the form $\binom{a\,0\,0}{0\,a\,0}$ with $1 \le a \le q$, and their reflection images. In the same way, we define the vertical double-plaquette $D_2 = C \cup (C + (0,1))$ and the associated event E_2. With these notations we have

$$\mathbf{Z}^2 \setminus \hat V(G) \subset \bigcup_{k=1}^{7} W_k \ ,$$

where the random subsets W_k of $\mathbf{Z}^2$ are given by

$$\begin{aligned} W_1 &= V(B_0) \ , \quad W_2 = V(B_0) - (1,0) \ , \quad W_3 = V(B_0) - (0,1) \ ,\\ W_4 &= \{i \in \mathcal{L}_{1,\rm even} : \sigma_{D_1+i} \in E_1\} \ , \quad W_5 = \{i \in \mathcal{L}_{1,\rm odd} : \sigma_{D_1+i} \in E_1\} \ ,\\ W_6 &= \{i \in \mathcal{L}_{2,\rm even} : \sigma_{D_2+i} \in E_2\} \ , \quad W_7 = \{i \in \mathcal{L}_{2,\rm odd} : \sigma_{D_2+i} \in E_2\} \ .\end{aligned}$$

(The sets W_k are not necessarily disjoint.) So, for each $\mu \in \mathcal{G}_{\rm per}(z,q)$ we can write

$$\mu(\Delta \cap \hat V(G) = \emptyset) \le \sum_{\Delta_1 \cup \ldots \cup \Delta_7 = \Delta} \min_{1 \le k \le 7} \mu(\Delta_k \subset W_k) \ , \tag{15}$$

where the sum extends over all disjoint partitions of Δ. We estimate now each term.

Consider first the case $k = 1$. Just as in Lemma 3.9 we obtain from the chessboard estimate

$$\mu(\Delta_1 \subset W_1)^{1/|\Delta_1|} \le \limsup_{L\to\infty} \frac{\mu^{z,q}_{L,\mathrm{per}}(B_{0,L})^{1/v(L)}}{\mu^{z,q}_{L,\mathrm{per}}(F_{1,L})^{1/v(L)}} = (zq)^{-1/4} ,$$

where $F_{1,L}$ is given by (14). The same estimate holds in the cases $k = 2, 3$ because these merely correspond to a translation.

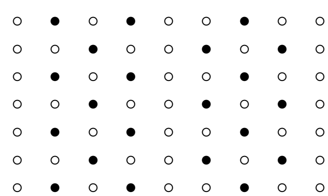
Next we turn to the case $k = 4$. Let L be so large that $\Lambda_L \supset \Delta_4$. Using reflection positivity in the lines through the sites of $\mathcal{L}_{1,\mathrm{even}}$, we conclude from the chessboard estimate that

$$\mu^{z,q}_{L,\mathrm{per}}(\Delta_4 \subset W_4)^{1/|\Delta_4|} \le \mu^{z,q}_{L,\mathrm{per}}(E_{1,L})^{2/v(L)}$$

for the event

$$E_{1,L} = \Big\{\sigma \in \Omega_{L,\mathrm{per}} : \sigma_{D_1(i)} \in E_1 \text{ for all } i \in \Lambda_L \cap \mathcal{L}_{1,\mathrm{even}}\Big\} .$$

In the above, $D_1(i)$ stands for the image $D_1 + i \bmod \Lambda_L$ of D_1 under the periodic shift by i of the torus Λ_L. Each $\sigma \in E_{1,L}$ has the following structure: every fourth vertical line (with horizontal coordinate either 0 or 2 modulo 4) is empty, and on each group of three vertical lines between these empty lines every second site is occupied, with the coordinates of occupied sites being either even-odd-even in these three lines, or odd-even-odd; see the figure below.



Of course, the interaction implies that the color of particles is constant in each of these groups of three vertical lines. Consequently, each such σ has particle number $3v(L)/8$, and $|E_{1,L}| = 2(2q)^{6L}$; recall the definition (6) of Λ_L.

We now make a construction similar to that in Lemma 3.7. We divide Λ_L into $12L^2$ rectangular cells $\Delta(j)$ of size 8×7. Let $\Delta_0(j)$ be the rectangular cell of size 7×6 situated in the left lower corner of $\Delta(j)$, and consider the set

$$F_L = \{\sigma \in \Omega_{L,\mathrm{per}} : \sigma_i \ne 0 \text{ iff } i_1 + i_2 \text{ is even and } i \in \Delta_0(j) \text{ for some } j\} .$$

Since $|\Delta(j) \setminus \Delta_0(j)| = |\Delta(j)|/4$ for all j, each $\sigma \in F_L$ has particle number $3\,v(L)/8$, just as the configurations in $E_{1,L}$. As the colors of the particles in the blocks $\Delta_0(j)$ can be chosen independently, we have $|F_L| = q^{12L^2} = q^{v(L)/56}$. Hence

$$\mu^{z,q}_{L,\mathrm{per}}(E_{1,L}) \le \frac{\mu^{z,q}_{L,\mathrm{per}}(E_{1,L})}{\mu^{z,q}_{L,\mathrm{per}}(F_L)} = \frac{|E_{1,L}|}{|F_L|} \le 2(2q)^{6L}\ q^{-v(L)/56}$$

and therefore, by taking the $2/v(L)$'th power and letting $L \to \infty$, we obtain

$$\mu(\Delta_4 \subset W_4)^{1/|\Delta_4|} \le q^{-1/28} .$$

The same estimate holds in the cases $k = 5, 6, 7$, as these are obtained by a translation or interchange of coordinates.

We now combine all previous estimates as follows. Let q_0 be so large that $7\,(q_0^{-1/28})^{1/7} < \delta$, and suppose that $q \geq q_0$ and $zq \geq q_0^{1/7}$. Then $\mu(\Delta_k \subset W_k) \leq q_0^{-|\Delta_k|/28}$ for all k and thus, in view of (15) and since $|\Delta_k| \geq |\Delta|/7$ for at least one k,

$$\mu(\Delta \cap \hat{V}(G) = \emptyset) \leq \sum_{\Delta_1 \cup \ldots \cup \Delta_7 = \Delta} (q_0^{-1/28})^{|\Delta|/7} < \delta^{|\Delta|}.$$

The proof of the contour estimate is therefore complete. □

To prove Theorem 2.3 we can now proceed as in Section 3.1. Let $\hat{S}(G)$ be the largest sea in $\hat{V}(G)$ if the latter contains a sea, and $\hat{S}(G) = \emptyset$ otherwise. It is then immediate that a counterpart of Proposition 3.2 holds, and the definition of $\hat{V}(G)$ implies that

$$\{\hat{S}(G) \neq \emptyset\} = \{\hat{S}(G_{\mathrm{dis}}) \neq \emptyset\} \cup \{\hat{S}(G_{\mathrm{ord}}) \neq \emptyset\}\ ,$$

where the two sets on the right-hand side are disjoint. Moreover,

$$\{\hat{S}(G_{\mathrm{ord}}) \neq \emptyset\} \subset \bigcup_{a=1}^{q} \{S(G_{a,\mathrm{even}}) \neq \emptyset\} \cup \{S(G_{a,\mathrm{odd}}) \neq \emptyset\}\ .$$

By the argument of Proposition 3.3 we thus obtain the existence of $2q$ ordered phases (as described in Theorem 2.3(i)) whenever z is such that $\mu(0 \in V(G_{\mathrm{ord}})) \geq \mu(0 \in V(G_{\mathrm{dis}}))$ for some $\mu \in \bar{\mathcal{G}}_{\mathrm{per}}(z, q)$, and the existence of a disordered phase μ_{dis} whenever the reverse inequality holds for such a μ. We have $\varrho(\mu_{\mathrm{dis}}) \leq \frac{1}{4} + \frac{3\varepsilon}{2}$ and $\varrho(\mu_{a,\mathrm{even}}) = \varrho(\mu_{a,\mathrm{odd}}) \geq \frac{1}{2} - \varepsilon$. The topological argument of Section 3.1 together with obvious counterparts of Lemmas 3.4 and 3.5 then show that both cases must occur simultaneously for some $z = z_c(q)$, and this z is unique by the convexity argument of Lemma 3.6. (For the latter we need to assume that $\varepsilon < 1/10$.)

We conclude this section with a comment on the model with nearest-particle color repulsion and a molecular hard-core exclusion between next-nearest neighbors.

Comment on Remark 2.3 (3). If the rôles of Φ and U are interchanged, the good ordered configurations in C are those with two particles of the same color on one side of C, and no particle on the opposite side; we call this set again G_{ord}. For large z, one can easily establish a contour estimate implying the existence of a sea $S(G_{\mathrm{ord}})$, and thus by symmetry also the existence of the four phases mentioned in Remark 2.3 (3). The disordered good plaquettes are again described by the set G_{dis}. As in the case of the Hamiltonian (4), the sets G_{ord} and G_{dis} have no disjoint side-projections. However, whereas in that case we were able to show an entropic disadvantage in having adjacent G_{ord}- and G_{dis}-plaquettes, this is not true in the present case. The configurations resulting from iterated reflections of a double plaquette of type $\binom{\circ\circ\circ}{\bullet\bullet\circ}$ have the maximal entropy possible for this particle number. Therefore the system can freely combine ordered and disordered plaquettes, and our argument for a first-order transition breaks down. So it seems likely that the transition from the ordered to the disordered phase is of second order.

6 Proof of Theorem 2.4

The analysis of the plane-rotor Widom–Rowlinson model is very similar to that of the standard Widom–Rowlinson model; only a few modifications are necessary. We define again the set Ω_C of admissible configurations in the plaquette C in the obvious way, introduce the sets $G_{\text{stag}} = G_{\text{even}} \cup G_{\text{odd}}$ as in Section 3.1 (replacing $\{1, \dots, q\}$ by S^1), and set $G_{\text{ord}} = \{\sigma \in \Omega_C : \sigma_i \in S^1 \text{ for all } i \in C\}$ and $G = G_{\text{ord}} \cup G_{\text{stag}}$. The main task is to obtain a counterpart of the contour estimate, Proposition 3.1. To this end we consider the same classes B_k, $k \in \{0, \dots, 3\}$ of bad configurations as in Section 3.2 (with the obvious modifications), and the sets $B_{k,L}$ and the associated quantities $p_k^{z,\alpha}$.

To deal with the case $k = 3$ we proceed as in Lemma 3.7, arriving at the inequality

$$\mu_{L,\text{per}}^{z,\alpha}(B_{3,L}) \le \frac{\mu_{L,\text{per}}^{z,\alpha}(B_{3,L})}{\mu_{L,\text{per}}^{z,\alpha}(F_{3,L})} = \frac{\nu^\Lambda(B_{3,L})}{\nu^\Lambda(F_{3,L})} .$$

Now, $\nu^\Lambda(B_{3,L}) \le 2^{14L+2}(2\alpha)^{3\,v(L)/4-1}$; the first factor estimates the number of possible occupation patterns, and the second term bounds the probability that the configuration is admissible (by keeping only the bonds in a tree spanning all occupied positions). On the other hand, $\nu^\Lambda(F_{3,L}) \ge (\alpha^{7\cdot 6-1})^{v(L)/56}$, as can be seen by letting the spins in each block $\Delta_0(k)$ follow a "leader spin" up to the angle $2\pi\alpha/2$. Hence

$$\frac{\nu^\Lambda(B_{3,L})}{\nu^\Lambda(F_{3,L})} \le 2^{14L+2}\ 2^{3\,v(L)/4}\ \alpha^{v(L)/56-1}$$

and therefore $p_3^{z,\alpha} \le 2^{3/4}\,\alpha^{1/56}$.

In the case $k = 2$ we proceed as in the proof of Lemma 3.8. On the one hand,

$$\nu^\Lambda(B_{2,L}) \le 2((2\alpha)^{24\,L-1})^{14\,L} + 2((2\alpha)^{28\,L-1})^{12\,L} \le 4(2\alpha)^{v(L)/2-14L}$$

since the spins are ordered in separate rows or columns, and $2\alpha < 1$. On the other hand, $\nu^\Lambda(F_{2,L}) \ge (\alpha^{2\cdot 3-1})^{v(L)/12}$ by the same argument as above. Hence

$$\mu_{L,\text{per}}^{z,\alpha}(B_{2,L}) \le \frac{\nu^\Lambda(B_{2,L})}{\nu^\Lambda(F_{2,L})} \le 4 \cdot 2^{v(L)/2}\ \alpha^{v(L)/12}\ (2\alpha)^{-14L}$$

and therefore $p_2^{z,\alpha} \le 2^{1/2}\,\alpha^{1/12}$.

Finally, for $k = 0$ we obtain

$$\mu_{L,\text{per}}^{z,\alpha}(B_{0,L}) \le \frac{\mu_{L,\text{per}}^{z,\alpha}(B_{0,L})}{\mu_{L,\text{per}}^{z,\alpha}(G_{\text{even},L})} = \frac{1}{z^{v(L)/2}}$$

and thus $p_0^{z,\alpha} \le z^{-1/2}$. Likewise, in the case $k = 1$ we get as in Lemma 3.9

$$\mu_{L,\text{per}}^{z,\alpha}(B_{1,L}) \le \frac{\mu_{L,\text{per}}^{z,\alpha}(B_{1,L})}{\mu_{L,\text{per}}^{z,\alpha}(G_{\text{even},L})} \le \frac{2^{14L+2} z^{v(L)/4}}{z^{v(L)/2}}$$

and thereby $p_1^{z,\alpha} \le z^{-1/4}$. Combining these estimates as in the proof of Proposition 3.1 we arrive at the counterpart of (7) as soon as α_0 is so small that

$$2^{3/4}\,\alpha_0^{1/56} + 2^{1/2}\,\alpha_0^{1/12} + \alpha_0^{1/4} + \alpha_0^{1/2} \le \delta$$

and $\alpha \le \alpha_0$, $z \ge 1/\alpha_0$.

To complete the proof of Theorem 2.4 as in Section 3.1 we still need to adapt Lemmas 3.4 and 3.5. Writing

$$\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{ord},L}) \le \frac{\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{ord},L})}{\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{even},L})} \le \frac{z^{v(L)}(2\alpha)^{v(L)-1}}{z^{v(L)/2}}$$

we find that for $z \le \alpha^{-2}/18$ and $\mu \in \bar{\mathcal{G}}_{\mathrm{per}}(z,\alpha)$

$$\mu\Big(0 \in V(G_{\mathrm{ord}})\Big) \le z^{1/2} 2\alpha \le 2/\sqrt{18} < (1-\delta)/2 \ .$$

Likewise, since

$$\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{stag},L}) \le \frac{\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{stag},L})}{\mu^{z,\alpha}_{L,\mathrm{per}}(G_{\mathrm{ord},L})} \le \frac{2\ z^{v(L)/2}}{z^{v(L)}\ \alpha^{v(L)-1}}\ ,$$

we see that for $z \ge 5\,\alpha^{-2}$ and $\mu \in \bar{\mathcal{G}}_{\mathrm{per}}(z,\alpha)$

$$\mu\Big(0 \in V(G_{\mathrm{stag}})\Big) \le z^{-1/2}\alpha^{-1} < (1-\delta)/2 \ .$$

The remaining arguments of Section 3.1 can be taken over with no change to prove Theorem 2.4.

References

[1] van den Berg, J. and Maes, C. (1994) Disagreement percolation in the study of Markov fields, *Ann. Probab.* **22**, 749–763.

[2] Brightwell, G.R., Häggström, O. and Winkler, P. (1998) Nonmonotonic behavior in hard-core and Widom–Rowlinson models, *J. Stat. Phys.* **94**, 415–435.

[3] Chayes, L., Kotecký, R. and Shlosman, S. (1995) Aggregation and intermediate phases in dilute spin systems, *Commun. Math. Phys.* **171**, 203–232.

[4] Chayes, L., Kotecký, R. and Shlosman, S. (1997) Staggered phases in diluted systems with continuous spins, *Commun. Math. Phys.* **189**, 631–640.

[5] Dobrushin, R.L. and Shlosman, S.B. (1981) Phases corresponding to minima of the local energy, *Selecta Math. Sov.* **1**, 317–338.

[6] Fröhlich, J. and Huckaby, D.A. (1985) Percolation in hard-core lattice gases and a model ferrofluid, *J. Stat. Phys.* **38**, 809–821.

[7] Fukuyama, M. (2000) Discrete symmetry breaking for certain short-range interactions, *J. Stat. Phys.*, to appear.

[8] Georgii, H.-O. (1988) *Gibbs Measures and Phase Transitions*, de Gruyter, Berlin New York.

[9] Georgii, H.-O., Häggström, O. and Maes, C. (2000) The random geometry of equilibrium phases, in: Domb and J.L. Lebowitz (eds.), *Phase Transitions and Critical Phenomena*, Academic Press.

[10] Kotecký, R. and Shlosman, S. (1982) First-order phase transitions in large entropy lattice systems, *Commun. Math. Phys.* **83**, 493–550.

[11] Lebowitz, J.L., Gallavotti, G. (1971) Phase transition in binary lattice gases, *J. Math. Phys.* **12**, 1129–1133.

[12] Lebowitz, J.L., Mazel, A., Nielaba, P., Šamaj, L. (1995) Ordering and demixing transitions in multicomponent Widom–Rowlinson models, *Phys.Rev.* **E 52**, 5985–5996.

[13] Nielaba, P., Lebowitz, J.L. (1997) Phase transitions in the multicomponent Widom–Rowlinson model and in hard cubes on the BCC-lattice, *Physica* **A 244**, 278–284.

[14] Ruelle, D. (1978) *Thermodynamic Formalism*, Addison-Wesley, Reading.

[15] Runnels, L.K., Lebowitz, J.L. (1974) Phase transitions of a multicomponent Widom–Rowlinson model, *J. Math. Phys.* **15**, 1712–1717.

[16] Widom, B. and Rowlinson, J.S. (1970) New model for the study of liquid-vapor phase transition, *J. Chem. Phys.* **52**, 1670–1684.